Uncertainty quantification of simulation codes based on experimental data

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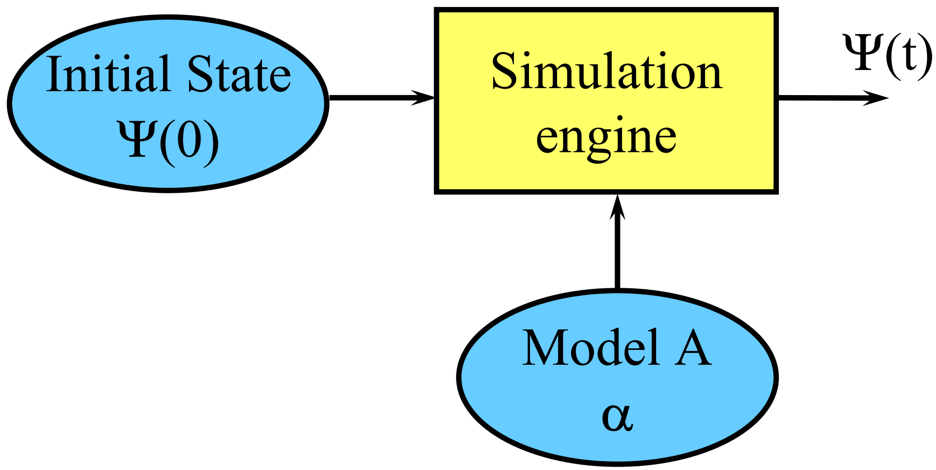
Overview

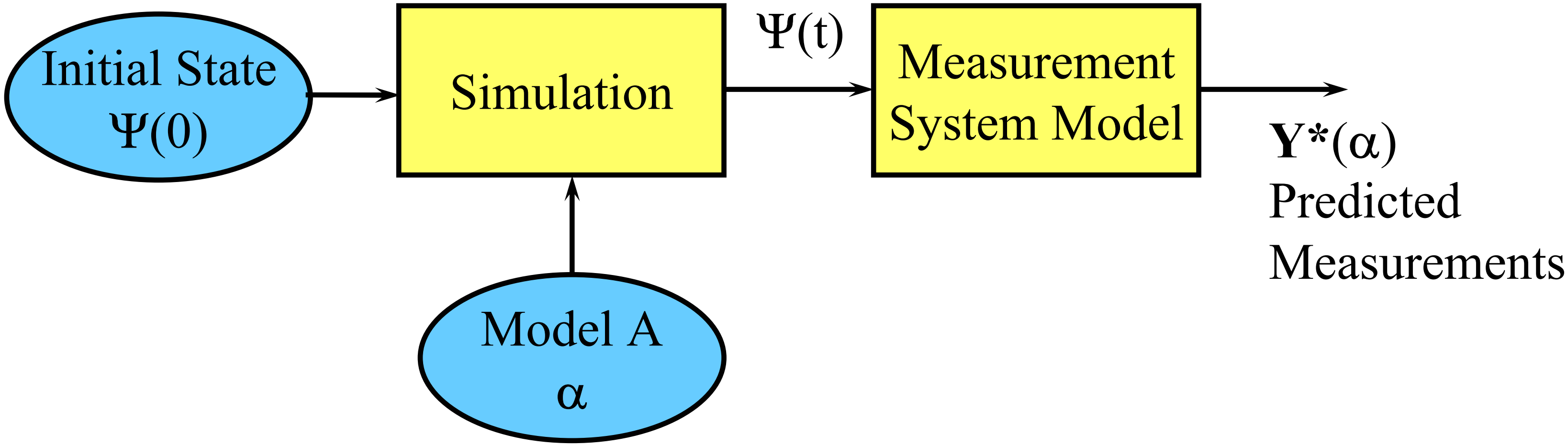
- Physics simulations codes
  - need to be understood on basis of experimental data
  - focus on physics submodels
- Bayesian analysis
  - more than parameter estimation
  - uncertainty quantification (UQ) is central issue
  - each new experiment used to improve knowledge of models
- Analysis process
  - employ hierarchy of experiments, from basic to fully integrated
  - goal is to learn as much possible from all experiments
- Example of analysis process: material model evolution

Schematic view of simulation code



- Simulation code predicts state of time-evolving system
  $\Psi(t)$ = time-dependent state of system
- Requires as input
  - $\Psi(0)$ = initial state of system
  - description of physics behavior of each system component; e.g., physics model A with parameter vector α (e.g., constitutive relations)
- Simulation engine solves the dynamical equations (PDEs)

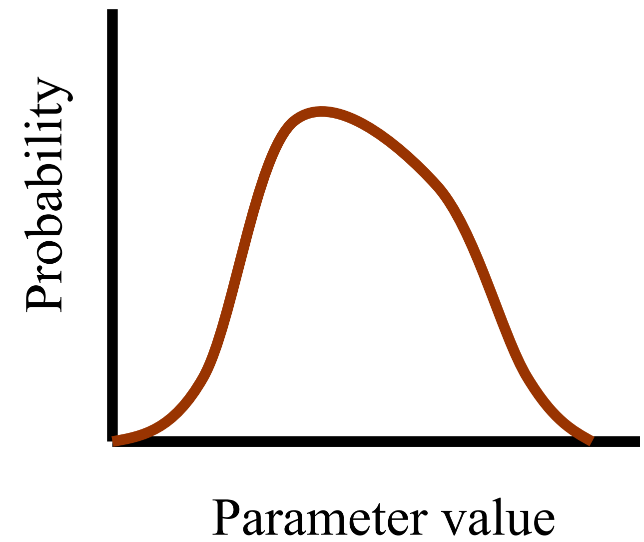
Simulation code predicts measurements



- Simulation code predicts state of time-evolving system
  $\Psi(t)$ = time-dependent state of system
- Model of measurement system yields predicted measurements

Bayesian uncertainty analysis

- Uncertainties in parameters are characterized by probability density functions (pdf)
- Probability interpreted as quantitative measure of "degree of belief"
- Rules of classical probability theory apply
- Bayes law provides way to update knowledge about models as summarized in terms of uncertainty

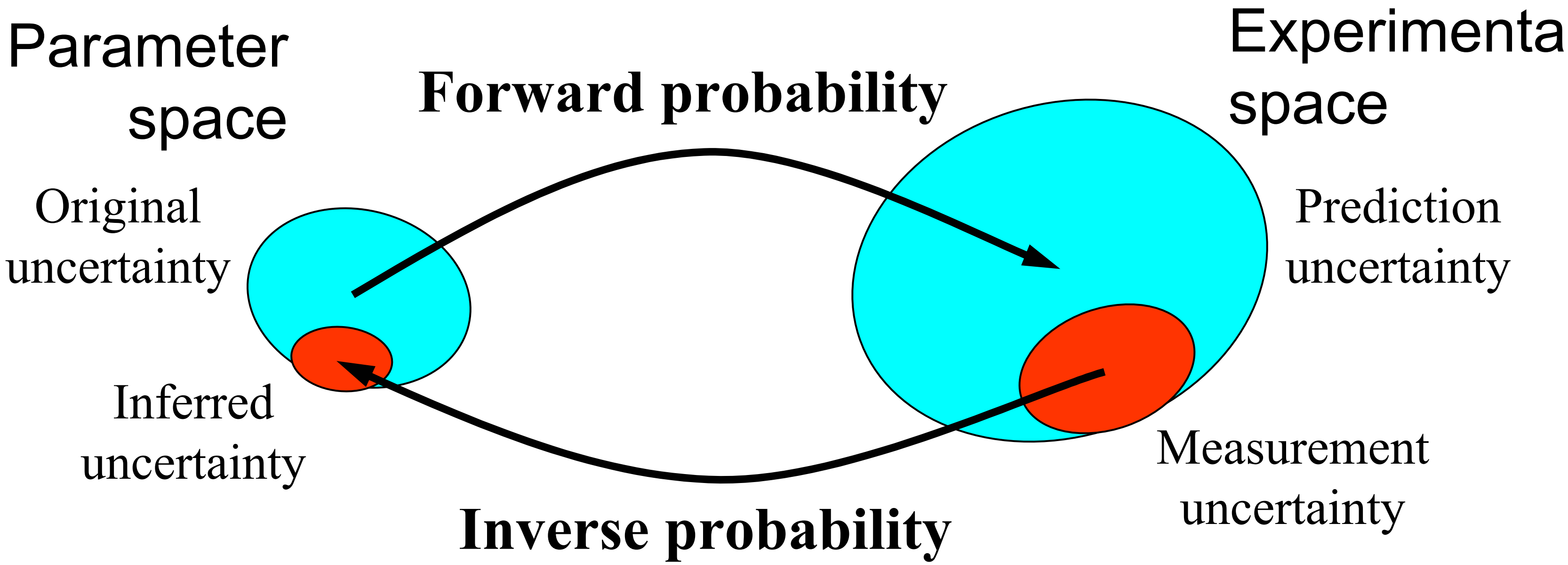


Bayesian calibration

Estimation of model parameters **and their uncertainties**

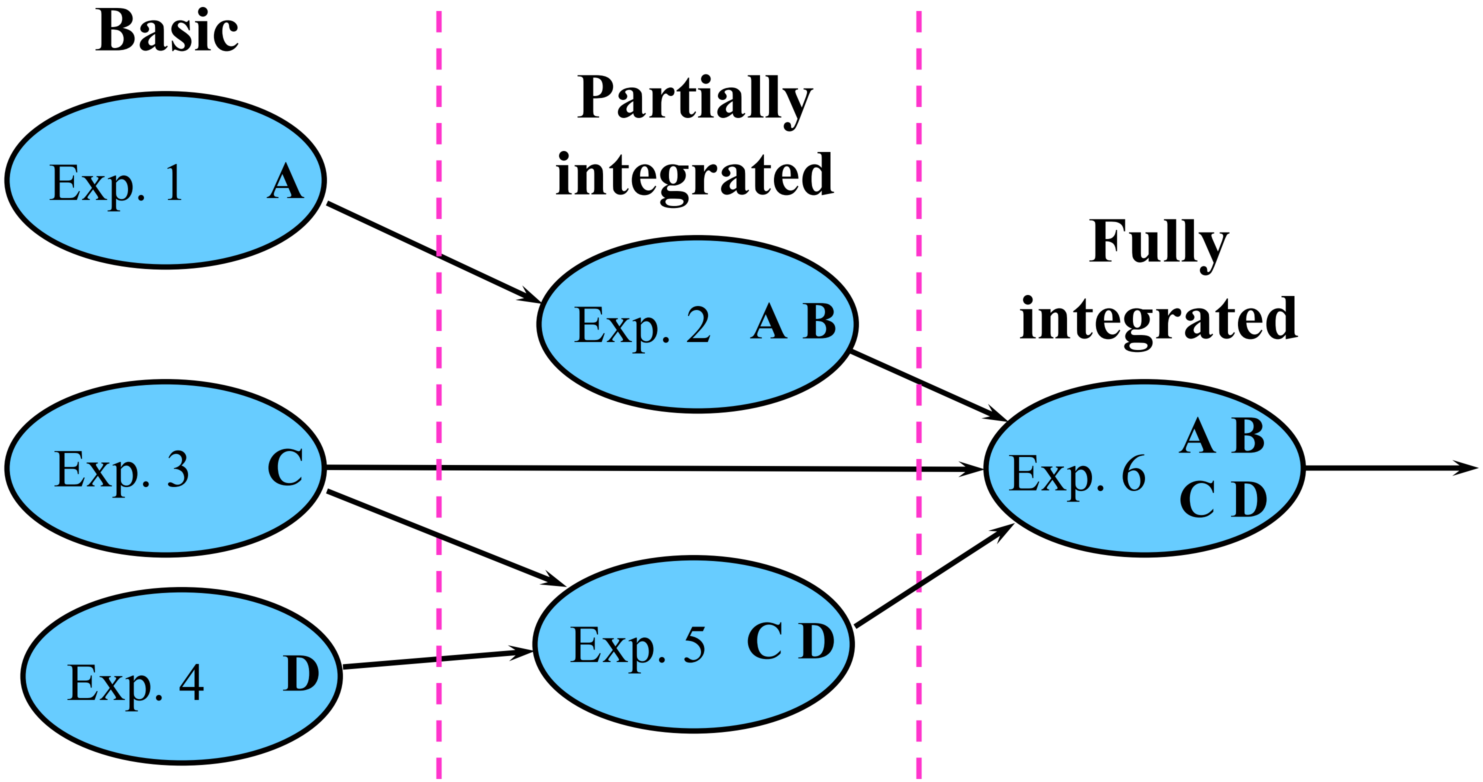
- Bayesian foundation
  - focus is as much on uncertainties in parameters as on their best value
  - use of prior knowledge, e.g., previous experiments
  - model checking;
    does model agree with experimental evidence?

Forward and inverse probability



- Model inference
  - if uncertainties in measurements are smaller than prediction uncertainties that arise from parameter uncertainties, one may be able to use measurements to reduce uncertainties in parameters
  - requires that prediction uncertainties are dominated by uncertainties in parameters and not by those in experimental set up
  - **good experimental technique** important for **Bayesian calibration**

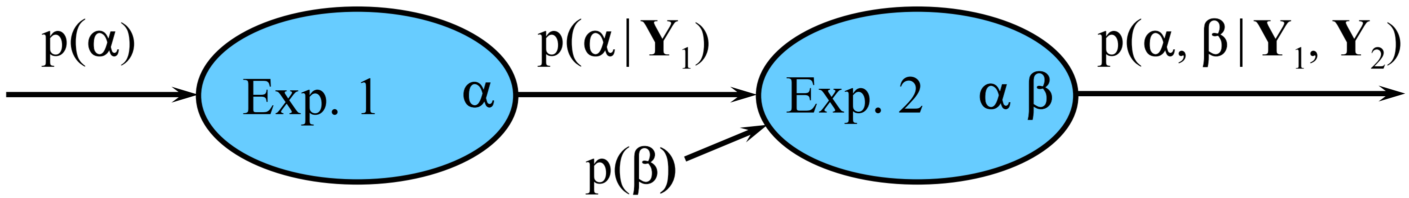
Analysis of hierarchy of experiments



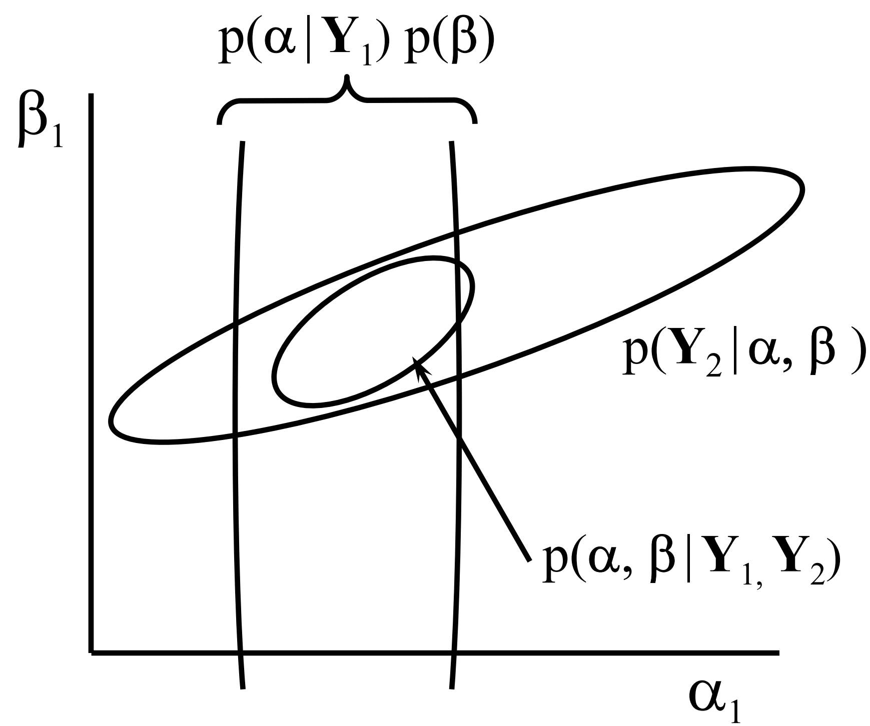
- Information flow in analysis of series of experiments
- Bayesian calibration –
  - analysis of each experiment updates model parameters and their uncertainties, consistent with previous analyses
  - information about models accumulates

Graphical probabilistic modeling

Propagate uncertainty through analyses of two experiments



- First experiment determines α, with uncertainties given by $p(\alpha \mid \mathbf{Y}_1)$
- Second experiment not only determines β but also refines knowledge of α
- Outcome is joint pdf in α and β, $p(\alpha, \beta \mid \mathbf{Y}_{1,} \mathbf{Y}_2)$ (NB: correlations)



Bayesian calibration for simulation codes

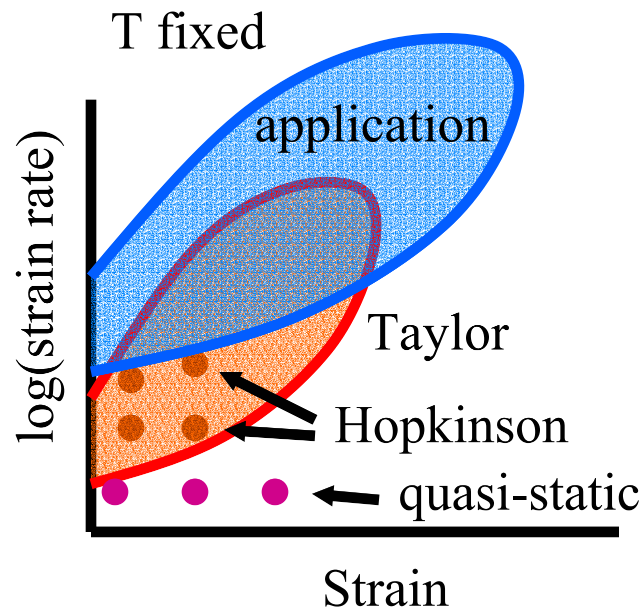
- Goal is to develop an uncertainty model for the simulation code by comparison to experimental measurements
  - determine and quantify sources of uncertainty
  - uncover potential inconsistencies of submodels with expts.
  - possibly introduce additional submodels, as required
- Recursive process
  - aim is to develop submodels that are consistent with all experiments (within uncertainties)
  - a hierarchy of experiments helps substantiate submodels over wide range of physical conditions
  - each experiment potentially advances our understanding

Motivating example

- Problem statement
  - design containment vessel using high-strength steel, HSLA 100
  - predict depth of vessel-wall penetration for specified shrapnel fragments at specified impact velocity
  - estimate uncertainty in this prediction to estimate safety factor
- Approach
  - determine what experiments are needed to characterize stress-strain relationship for plastic flow of metal
  - follow the uncertainty through the analysis of expt. data
  - variables to consider: temperature, strain rate, variability in material composition, processing, behavior

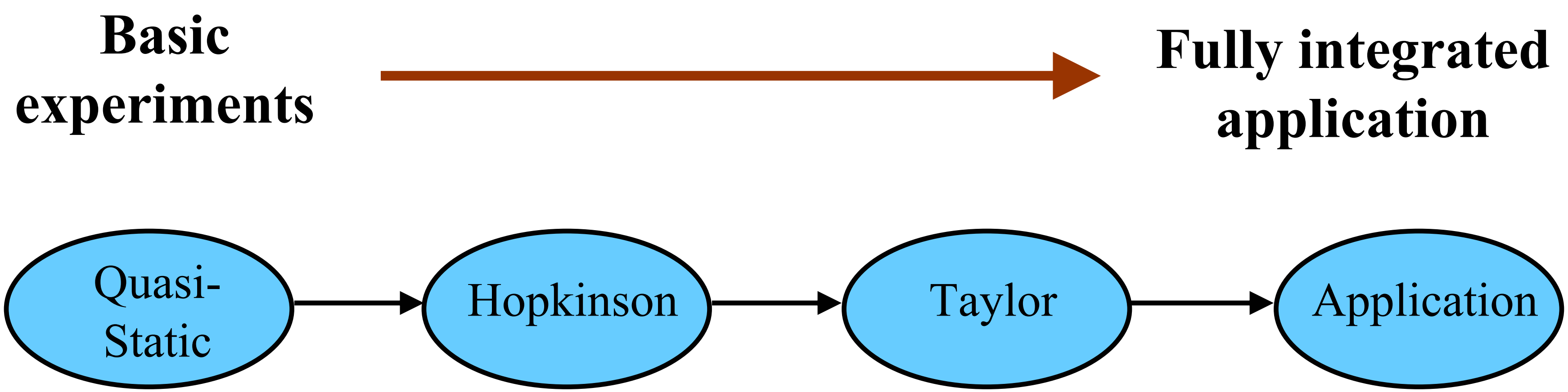
Hierarchy of experiments - plasticity

- Basic characterization experiments - measure stress-strain relationship at specific stain and strain rate
  - quasi-static – low strain rates
  - Hopkinson bar – medium strain rates



- Partially integrated expts. - Taylor test
  - covers range of strain rates
  - extends range of physical conditions
- Full integrated expts.
  - mimic application as much as possible
  - **projectile impacting plate**
  - may involve extrapolation of operating range; so introduces addition uncertainty
  - integrated expts. can help reduce model uncertainties

Analysis of hierarchy of experiments



- Series of experiments to determine plastic behavior of a metal
- Information flow shown for analysis sequence
- Bayesian calibration –
  - analysis of each experiment updates model parameters and their uncertainties, consistent with previous experiments
  - information about models accumulates throughout process

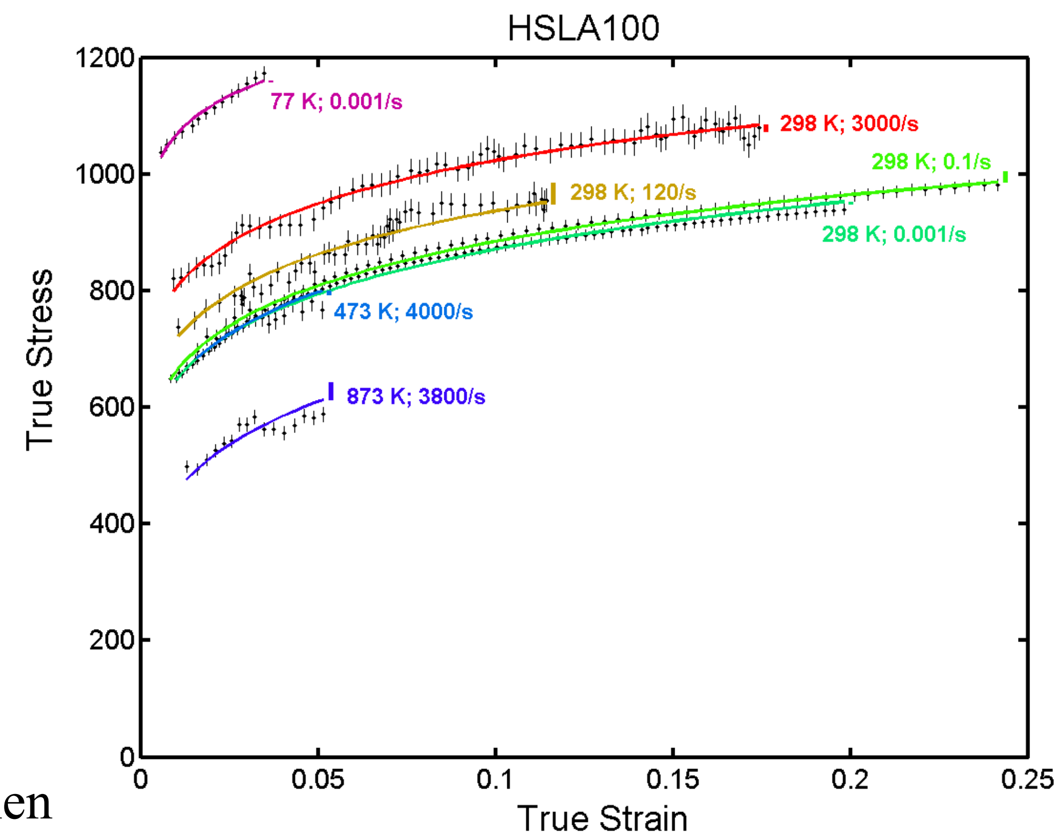
Stress-strain relation for plastic deformation

Analysis of quasi-static and Hopkinson bar measurements†

- Zerilli-Armstrong model for rate- and temperature-dependent plasticity

$$\sigma = \alpha_1 + \alpha_5 \varepsilon_p^{\alpha_6} + \alpha_2 \exp\left[\left(-\alpha_3 + \alpha_4 \log \frac{\partial \varepsilon_p}{\partial t}\right) T\right]$$

- Parameters determined from Hopkinson bar measurements and quasi-static tests
- Full uncertainty analysis – including systematic effects of offset of each data set (6 + 7 parms)



†data supplied by Shuh-Rong Chen

ZA parameters and their uncertainties

Parameters +/- rms error:

$\alpha 1 = 103 \pm 33$

$\alpha 2 = 954 \pm 63$

$\alpha 3 = 0.00408 \pm 0.00059$

$\alpha 4 = 0.000117 \pm 0.000029$

$\alpha 5 = 996 \pm 22$

$\alpha 6 = 0.247 \pm 0.021$

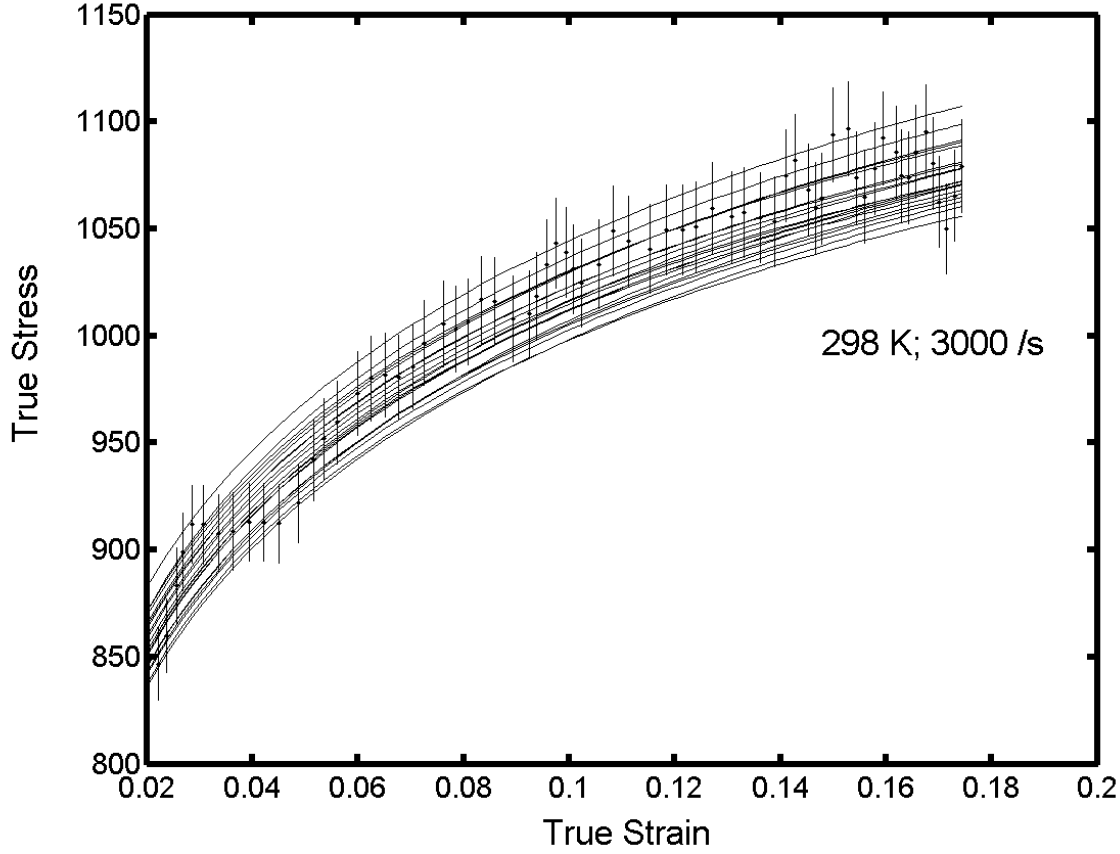
RMS errors, including correlation coefficients, crucially important!

Correlation coefficients

	α1	α2	α3	α4	α5	α6
α1	1	-0.083	0.372	0.207	-0.488	0.267
α2	-0.083	1	0.344	0.311	0.082	0.130
α3	0.372	0.344	1	0.802	0.453	-0.621
α4	0.207	0.311	0.802	1	0.271	-0.466
α5	-0.488	0.082	0.453	0.271	1	-0.860
α6	0.267	0.130	-0.621	-0.466	-0.860	1

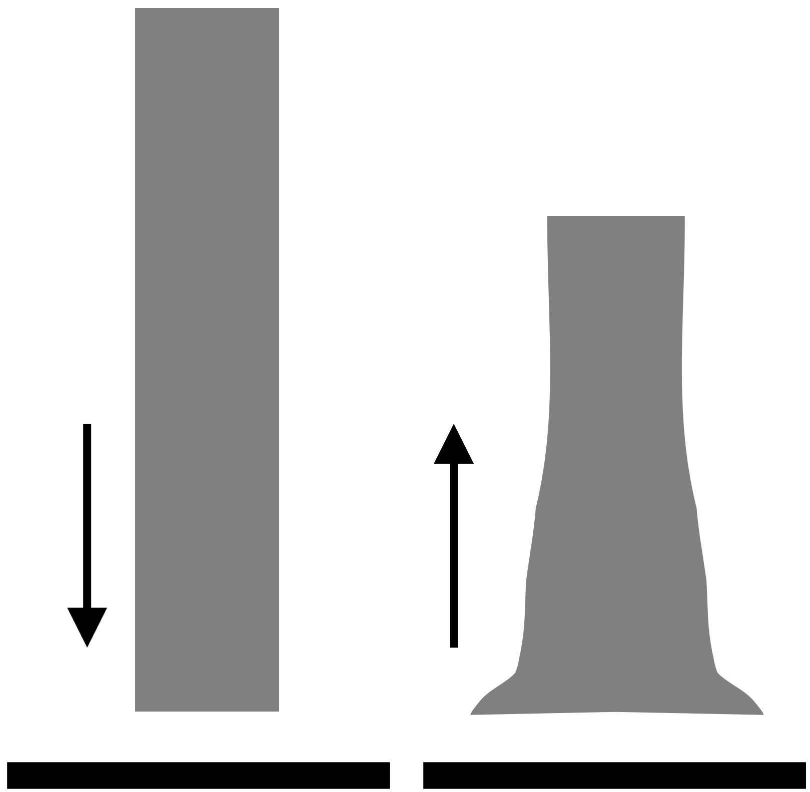
Monte Carlo sampling

- Use Monte Carlo to draw random samples from uncertainty distribution for Zerilli-Armstrong parameters



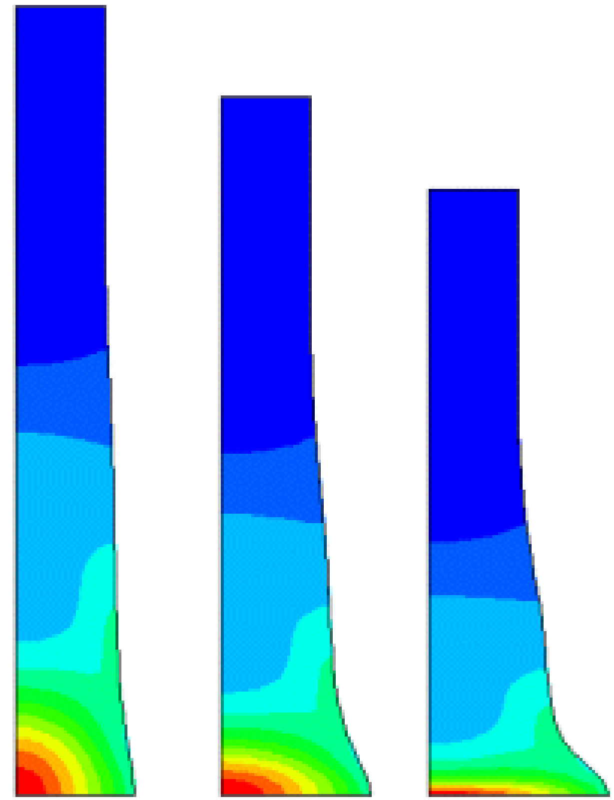
Taylor impact test

- Propel cylinder into rigid plate
- Measure profile of deformed cylinder
- Deformation depends on
  - cylinder dimensions
  - impact velocity
  - plastic flow behavior of material at high strain rate
- Useful for
  - determining parameters in material-flow model
  - validating simulation code (including material model)



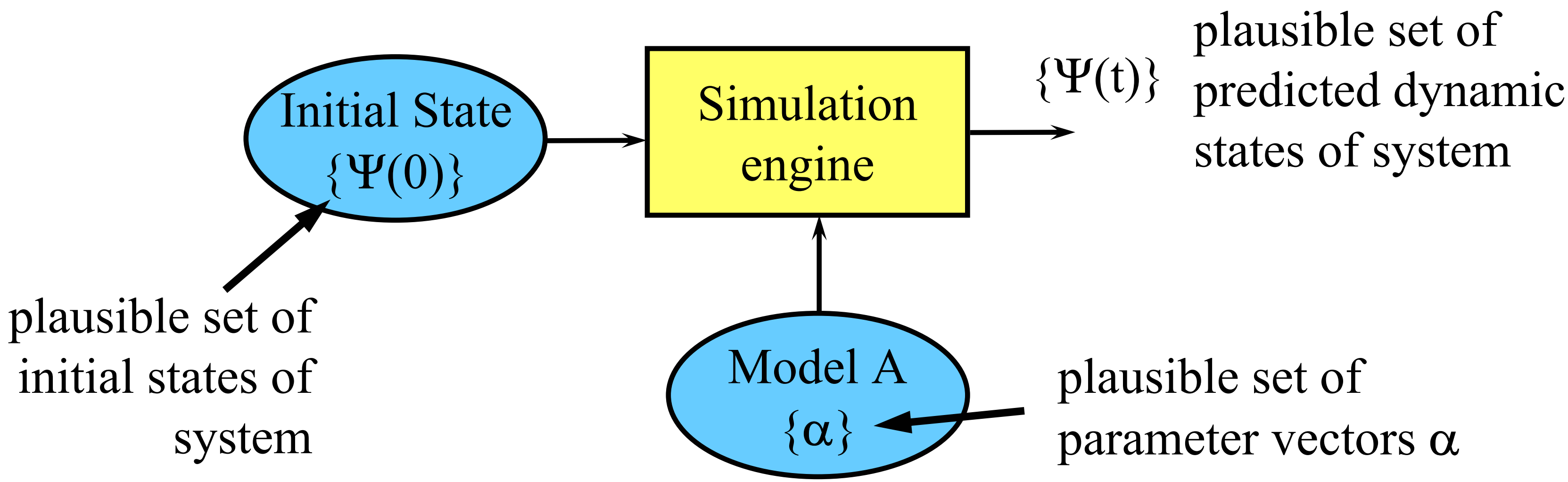
Taylor test simulations

- Simulate Taylor impact test
  - Abaqus, commercial FEM code
  - Johnson-Cook model for rate-dependent strength and plasticity
  - ignore anisotropy, fracture effects
  - cylinder: high-strength steel
    15-mm dia, 38-mm long
  - impact velocity = 350 m/s
- Effective total strain reaches 250%



17 μs   33 μs   50 μs

Plausible simulation predictions (forward)

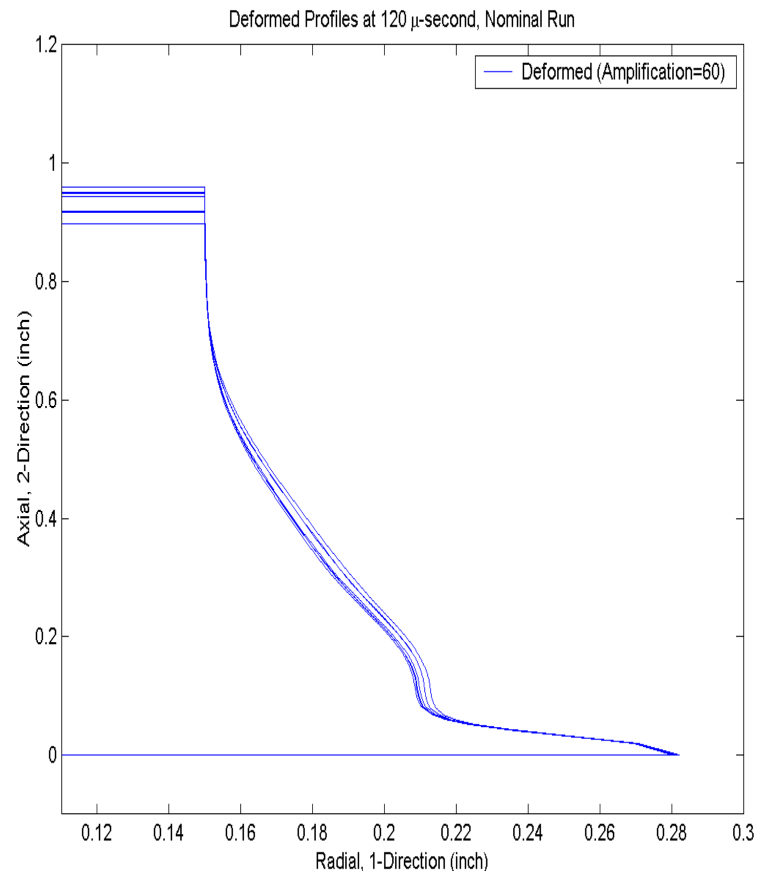


- Generate plausible predictions for known uncertainties in parameters and initial conditions
- Monte Carlo method
  - run simulation code for each random draw from pdf for α, $p(\alpha\,|.)$, and initial state, $p(\Psi(0)\,|.)$
  - simulation outputs represent plausible set of predictions, $\{\Psi(t)\}$

Monte Carlo example - Taylor test

- Use MC technique to propagate uncertainties through deterministic simulation code
  - Draw value for each of four parameters from its assumed Gaussian pdf
  - Run Abaqus code for each set of parameters
- Figure shows range of variation in predicted cylinder shape

NESSUS/Abaqus



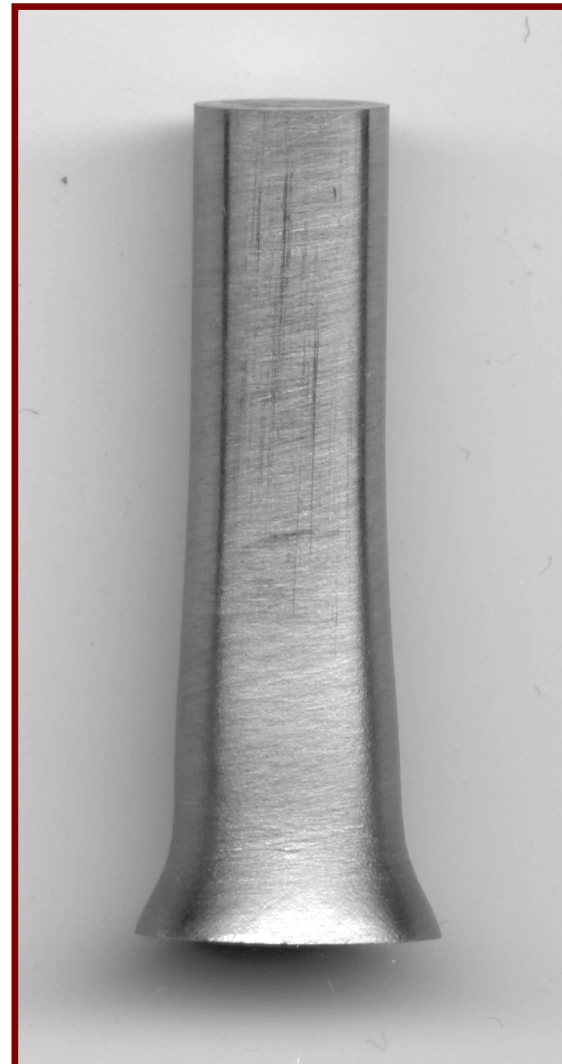
High-strength steel HSLA 100
246 m/s impact velocity

Taylor test experiment

- Taylor impact test specimen
  - high-strength steel HSLA 100
  - impact velocity = 245.7 m/s
  - dimensions, final/initial

    length 31.84 mm / 38 mm

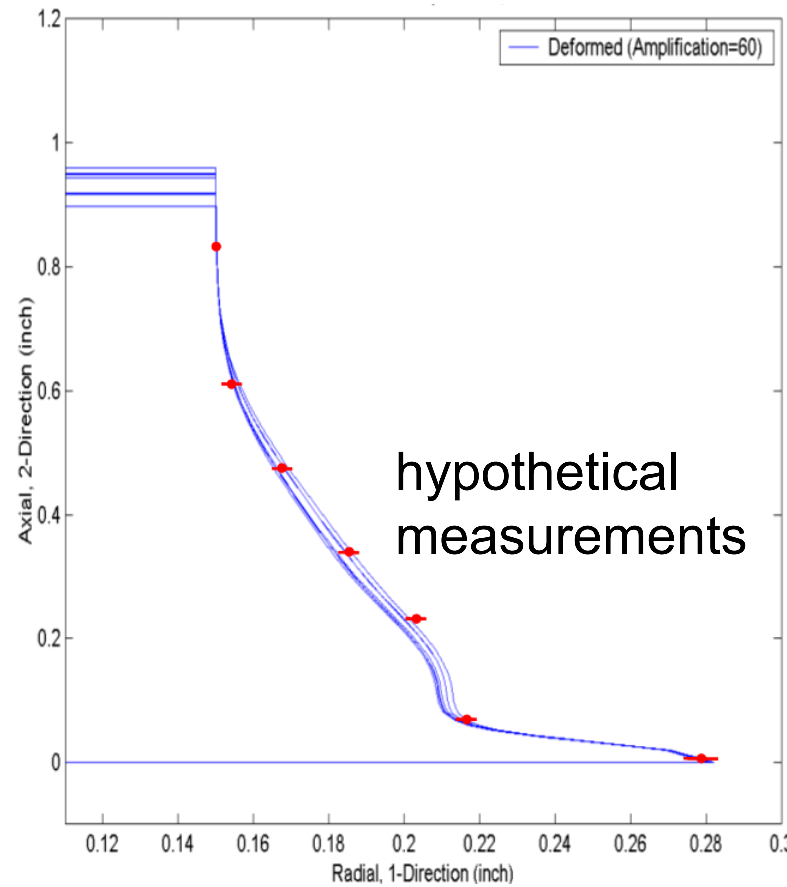
    diameter 12.00 mm / 7.59 mm



Comparison with experiment

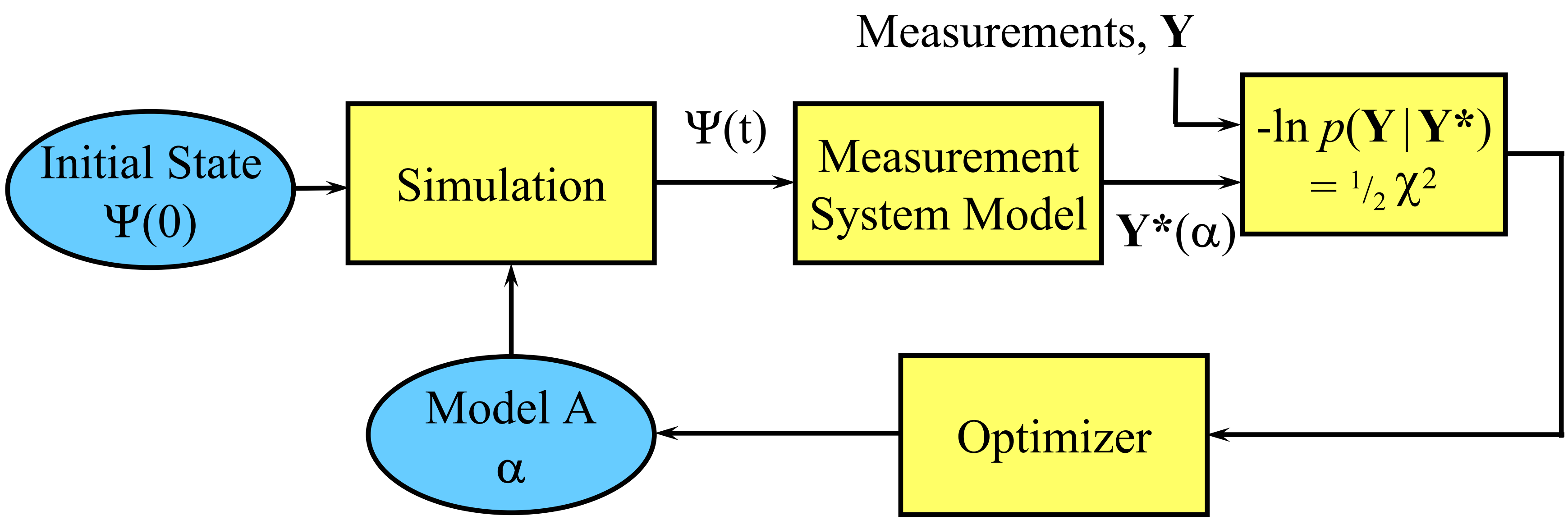
- Don't have measurements of the deformed cylinder yet, but suppose we do
- ZA model parameters can be fit to Taylor data in same way as they were to basic material characterization data
- Results of previous analysis may be used as prior in this analysis

NESSUS/Abaqus



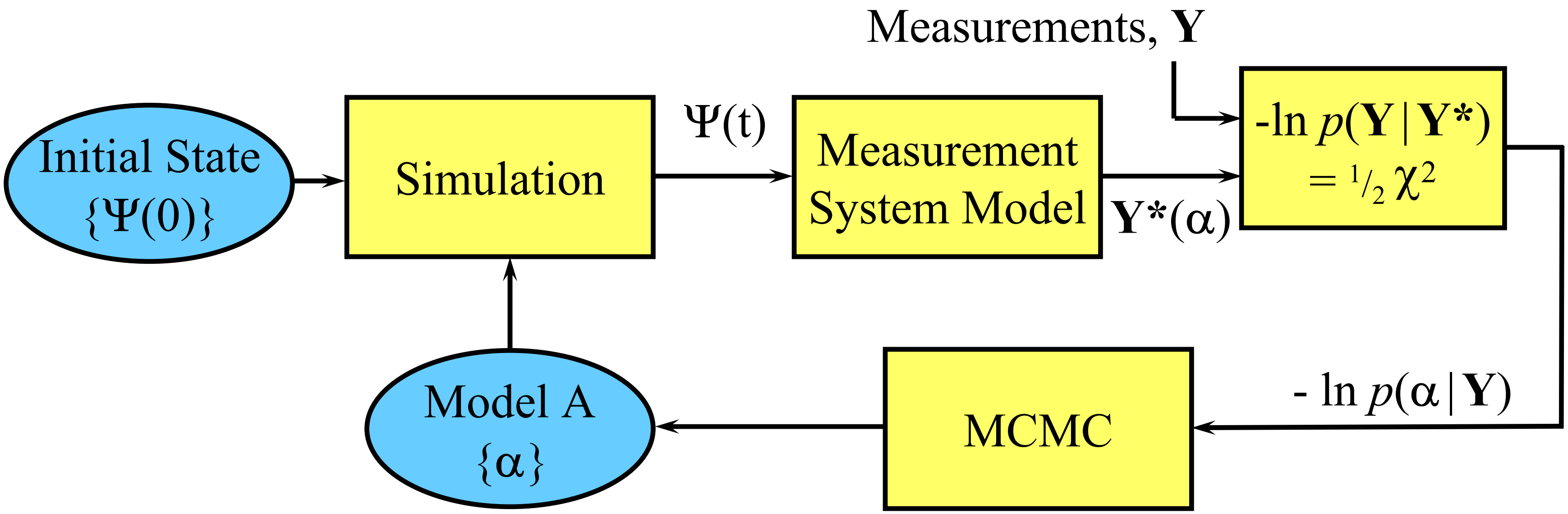
High-strength steel HSLA 100
246 m/s impact velocity

Parameter estimation - maximum likelihood



- Optimizer adjusts parameters (vector α) to minimize -ln $p(\mathbf{Y} \mid \mathbf{Y}^*(\alpha))$
- Result is maximum likelihood estimate for α (also known as minimum-chi-squared solution)
- Optimization process is accelerated by using gradient-based algorithms along with adjoint differentiation to calculate gradients of forward model

Parameter uncertainties via MCMC



- Markov Chain Monte Carlo (MCMC) algorithm generates a random sequence of parameters that sample posterior probability of parameters for given data **Y**, $p(\alpha \mid \mathbf{Y})$, which yields plausible set of parameters $\{\alpha\}$.
- Must include uncertainty in initial state of system, $\{\Psi(0)\}$

Bayesian strategy for UQ of simulation code

- Hierarchy of experiments
  - basic - designed to isolate and characterize a basic physical phenomenon at single
  - partially integrated - involves more complex combination of phenomena, e.g., multiple materials, varying conditions, complex geometry, ...
  - fully integrated - attempt to approach application conditions
- Inference - use validation experiments to update info about model
  - capture info in terms of uncertainties
  - uncertainties indicate degree of confidence in prediction
  - attempt to develop model that is consistent with ALL available experiments
- Ultimate goal - Combine results from many (all) experiments
  - reduce uncertainties in model parameters
  - require consistency of models with all experiments

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- "Inversion based on complex simulations," K. M. Hanson, *Maximum Entropy and Bayesian Methods*, pp. 121-135 (Kluwer Academic, 1998); describes adjoint differentiation and its usefulness in simulation physics
- "Uncertainty assessment for reconstructions based on deformable models," K. M. Hanson et al., *Int. J. Imaging Syst. Technol.* **8**, pp. 506-512 (1997); use of MCMC to sample posterior

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